

2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester
13533-05-6 | DTXSID5050397

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.89 | 0.25 | 0.88 | 0.26 | 0.75 | 0.38 |

Model Results

Predicted value: 4.13 days

Global applicability domain: Outside

Local applicability domain index: 2.51e-01

Confidence level: 8.16e-01

Nearest Neighbors from the Training Set

| | | |
|-----------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------|
| <div>Image not found</div> <div>2-Methylhexane</div> <div>Measured: 12.5</div> <div>Predicted: 5.54</div> | <div>Image not found</div> <div>2-Methylheptane</div> <div>Measured: 12.5</div> <div>Predicted: 3.99</div> | <div>Image not found</div> <div>2-Methyloctane</div> <div>Measured: 40.7</div> <div>Predicted: 4.23</div> |
| <div>Image not found</div> <div>3-Methylhexane</div> <div>Measured: 157</div> <div>Predicted: 6.83</div> | | |